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ABSTRACT

This document outlines the operation of the Monte Carlo Integration Computer (MCIC), which is capable of simulating several types of chemical processes. Some data obtained through the MCIC simulation of physical processes are presented in graphs. After giving reasons for not using the initially contemplated summative research procedures for evaluation of the MCIC as a teaching aid, the author chooses to use a diagnostic or formative evaluation. Evaluation occurred over three lecture/demonstrations of the MCIC to high school chemistry students in Philadelphia. Sample findings from one problem area - understanding the presentation of the MCIC - were presented to illustrate that formative evaluation of instructional materials might be more profitable than more traditional evaluations. (JM)

ED 065303

THE DEVELOPMENT AND DIAGNOSTIC EVALUATION OF THE MONTE CARLO INTEGRATION COMPUTER AS A TEACHING AID

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The research presented herein represents a portion of a dissertation study completed within the College of Education, Section of Science Education, Temple University, summer 1971.

DEVELOPMENT

A special-purpose digital computer has been developed that utilizes the Monte Carlo integration method for obtaining simulations of chemical processes. The computer, designated as the Monte Carlo Integration Computer (MCIC) is designed as an instructional aid for the illustration of kinetic and equilibrium processes. The MCIC is capable of quantitatively simulating microscopic, macroscopic, first-order, second-order, consecutive and catalytic kinetic processes and microscopic, macroscopic, Le Chatelier and catalytic equilibrium processes. The MCIC is illustrated in Figure 1.

Rationale of Operation

The MCIC contains input, memory, control, logic and output circuitry similar in function to conventional digital computers. The computer contains three memory arrays designated A, B and C. Each array contains 49 memory cells that are capable of existing in one of two states: "on" or "off." The state of each cell is indicated by a specific panel lamp on the MCIC display board. If, for example, 25 memory cells within the "B" array are in an "on" state, then 25 lamps within panel array "B" will be lit. The MCIC display board, therefore, continuously indicates the state of each memory cell within each array.

Each panel lamp analogously represents the existence or non-existence of a single atomic or molecular reacting particle. If, as in the above example, 25 panel lamps within the B array are lit, then 25 particles of "B" are represented. Each array can be thought of as representing a "reaction flask" containing a specific reacting species. Concentration meters located below the panel array lamps add or "integrate" the number of memory cells in the "on" condition and convert to appropriate concentration units.

Switching circuitry within the MCIC randomly connects individual memory cells within a given array to logic circuitry. The logic circuitry performs specified operations upon the connected memory cells. Simulating the reaction

$$A \longrightarrow B$$

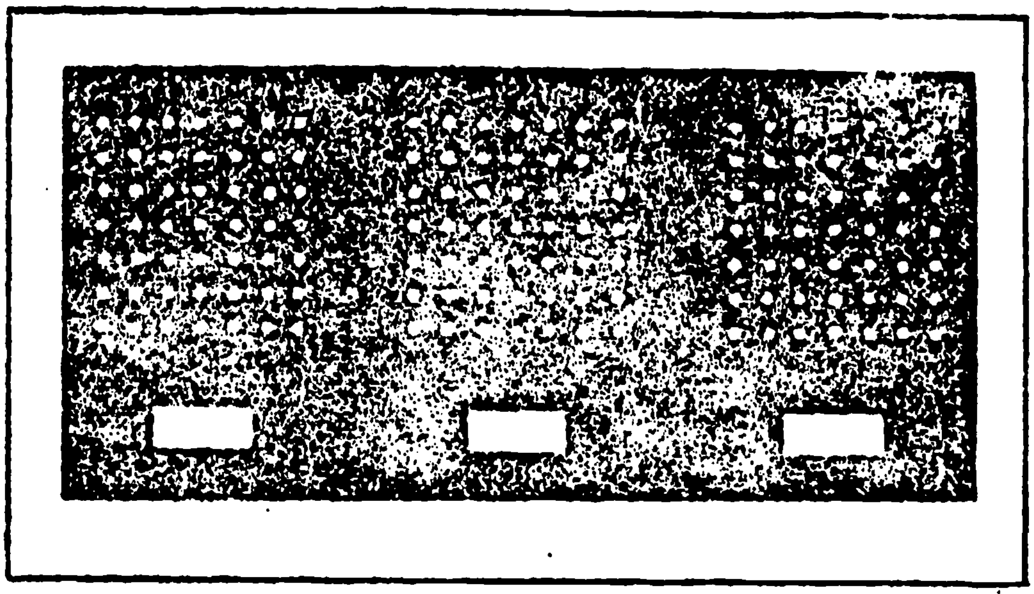
for example, requires the switching mechanism to randomly select a cell within the "A" array and connect it to the appropriate logic circuitry. If the located memory cell is in the "on" state, the logic circuitry turns the cell "off" and turns a "B" cell "on" that was previously in the "off" state. The above process therefore analogously represents the transformation of a particle of reactant "A" into a particle of product "B."

The reaction process is repeated by the switching circuitry randomly selecting a second "A" memory cell. If, by chance, a cell is selected that is in the "off" state, the logic circuitry allows the cell to remain in the "off" state, thereby indicating no reaction. It should be noted that the operation of the switching circuitry to produce specific rate-orders is dependent upon the ability of the switching circuitry to locate memory cells in a random manner. The first-order decreases in reaction rate with time, for example, must result from the increased random selection of some cells that have previously been switched off.

A "clock" mechanism within the MCIC indicates machine time. Unit intervals of machine time vary in duration, however, their average is proportional to "real" time. Simulated MCIC reaction processes can be started and stopped at will thus facilitating the recording and plotting of simulated reactions as a function of machine time. Such plots can be utilized for the calculation of rate constants and orders.

Equilibrium processes can be simulated by programming the MCIC in such a manner that a reaction and its reverse are coupled. Equilibrium constants can be calculated by determining the concentration of species at equilibrium.

In summary, both microscopic and macroscopic aspects of reaction processes are simulated through the utilization of percent concentration meters to indicate the changing concentrations of reaction species and panel display lamps to indicate the reaction processes occurring for individual reaction species. Data obtained through the MCIC simulation of physical processes is presented in Figure 2 through Figure 6. The data closely follows calculated values for first-order, second-order, consecutive, catalyzed, and equilibrium systems. In addition, equations that describe the MCIC's program of operations approximate chemical kinetic equations for both microscopic and macroscopic level processes.



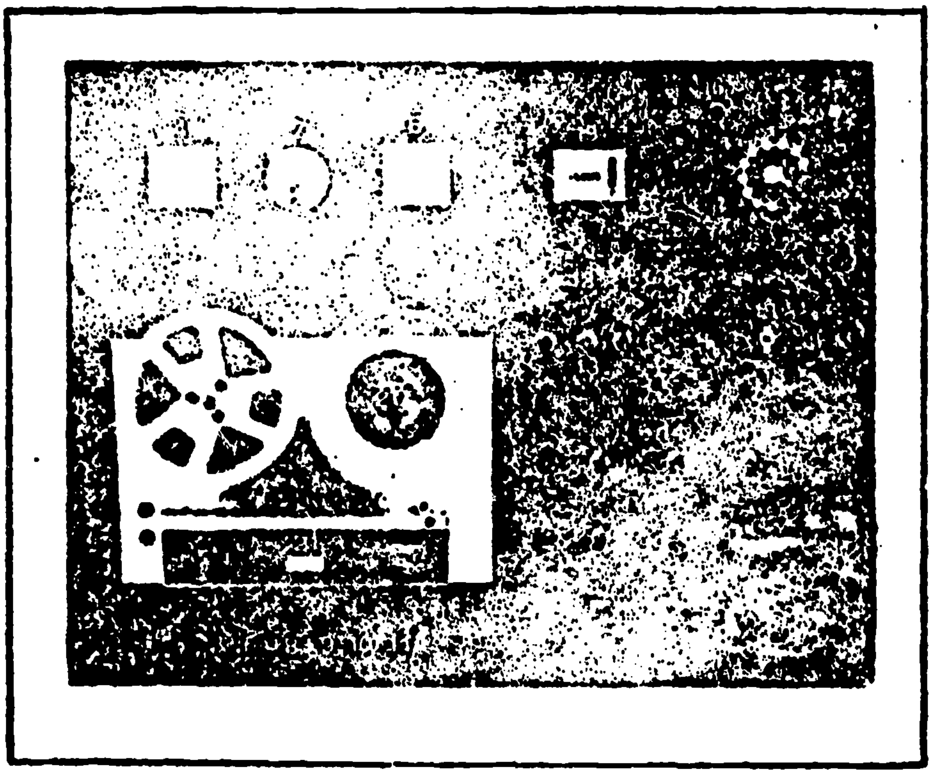


FIGURE 2
MCIC DISPLAY PANEL

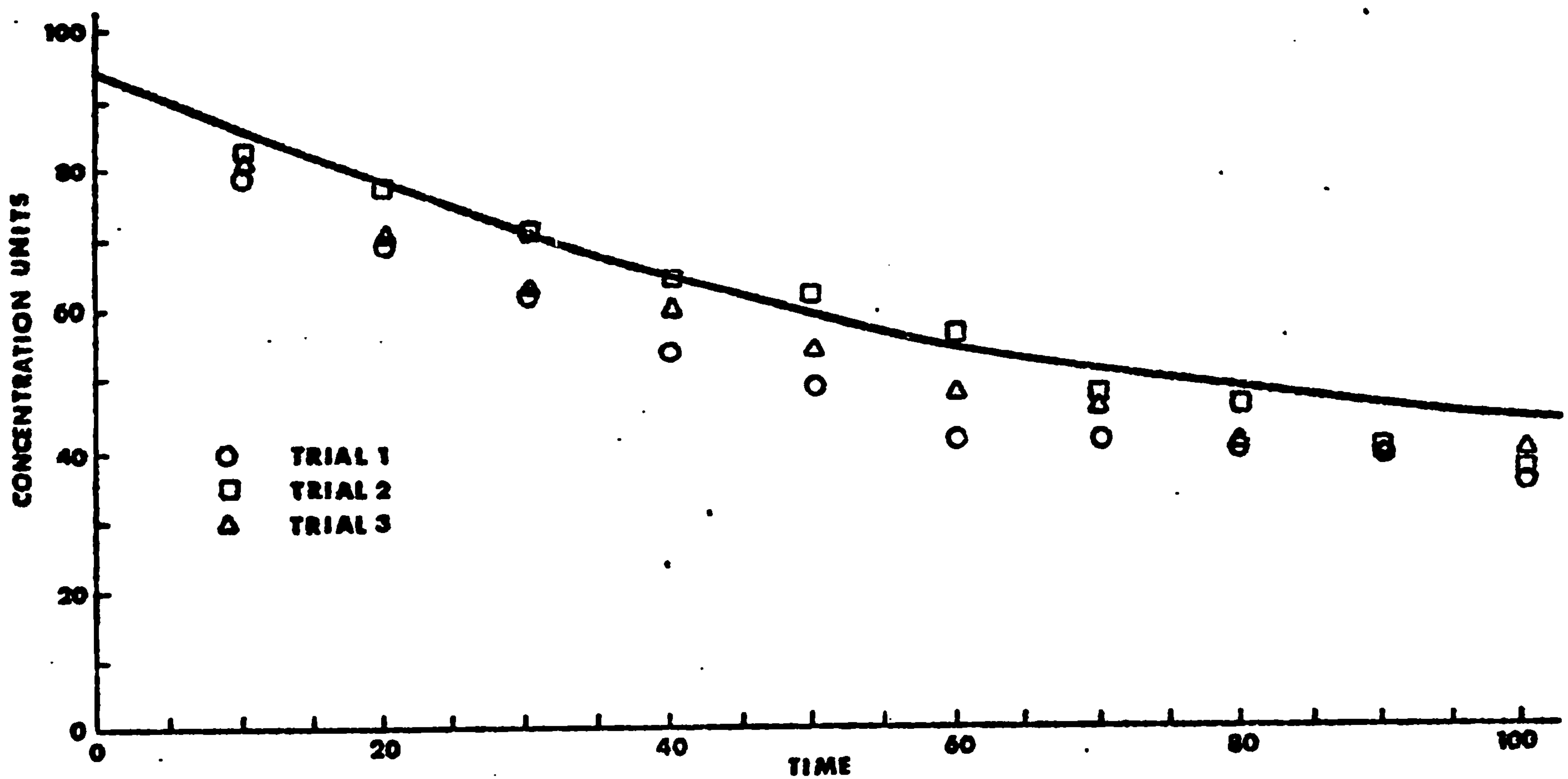


FIGURE 2
DEPEDENCE OF REACTANT CONCENTRATION UPON TIME FOR CHEMICAL AND MCIC SIMULATED SECOND-ORDER PROCESSES

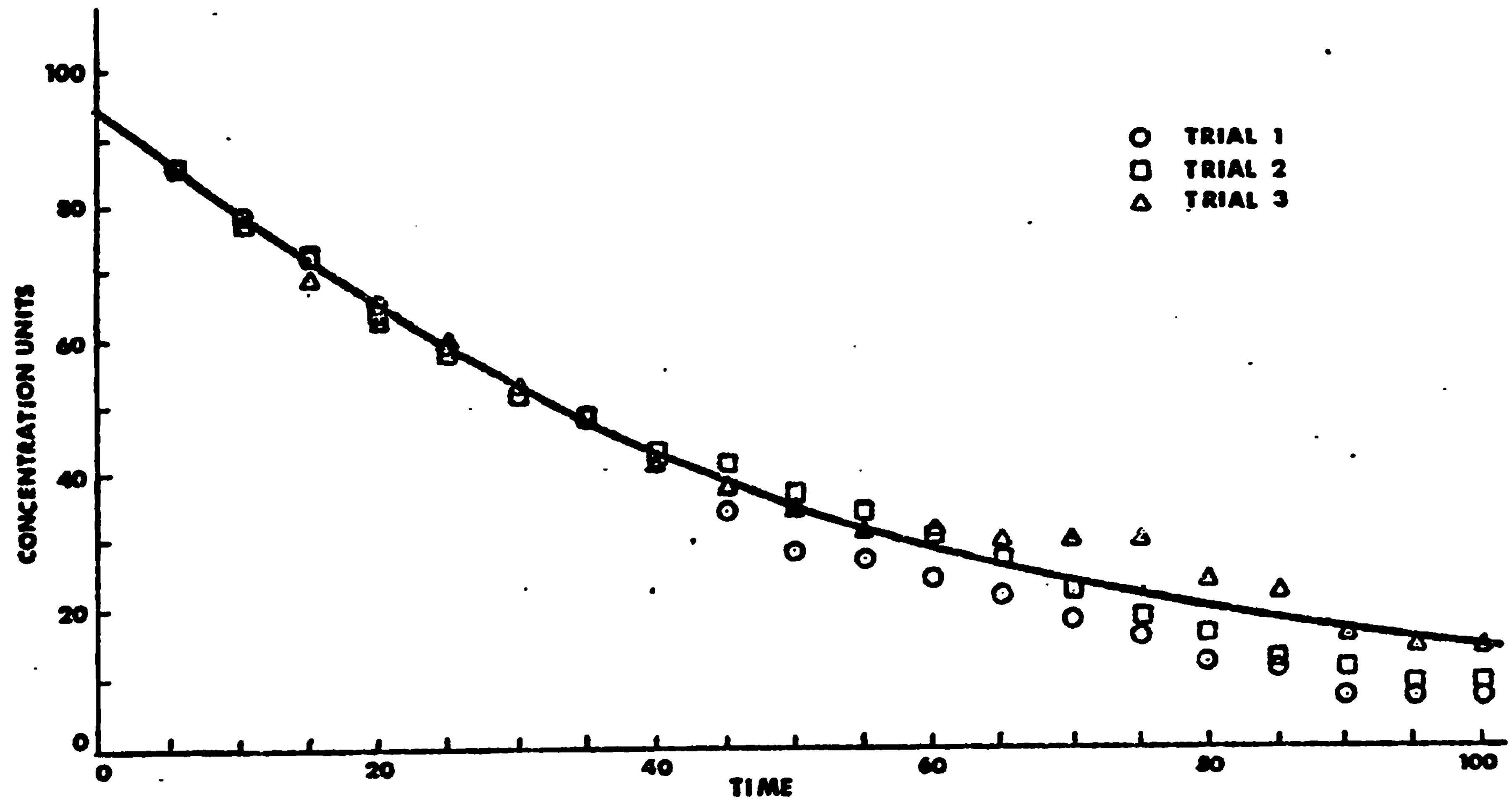


FIGURE 3
DEPENDENCE OF REACTANT CONCENTRATION UPON TIME FOR CHEMICAL AND MCIC SIMULATED FIRST-ORDER PROCESSES

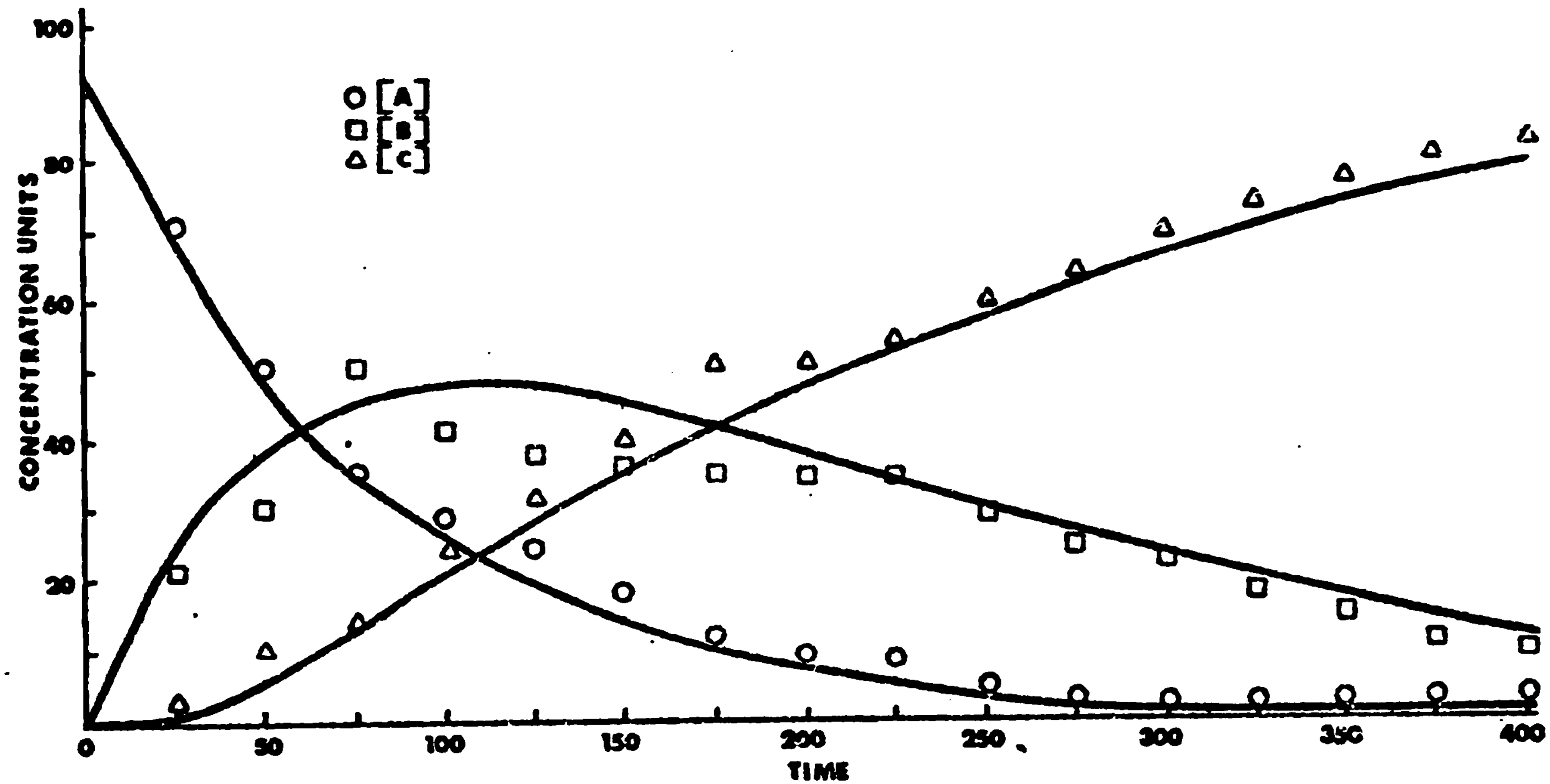


FIGURE 4
DEPENDENCE OF REACTANT CONCENTRATION UPON TIME FOR CHEMICAL AND MCIC SIMULATED FIRST-ORDER CONSECUTIVE PROCESSES OF THE FORM $A \rightarrow B \rightarrow C$

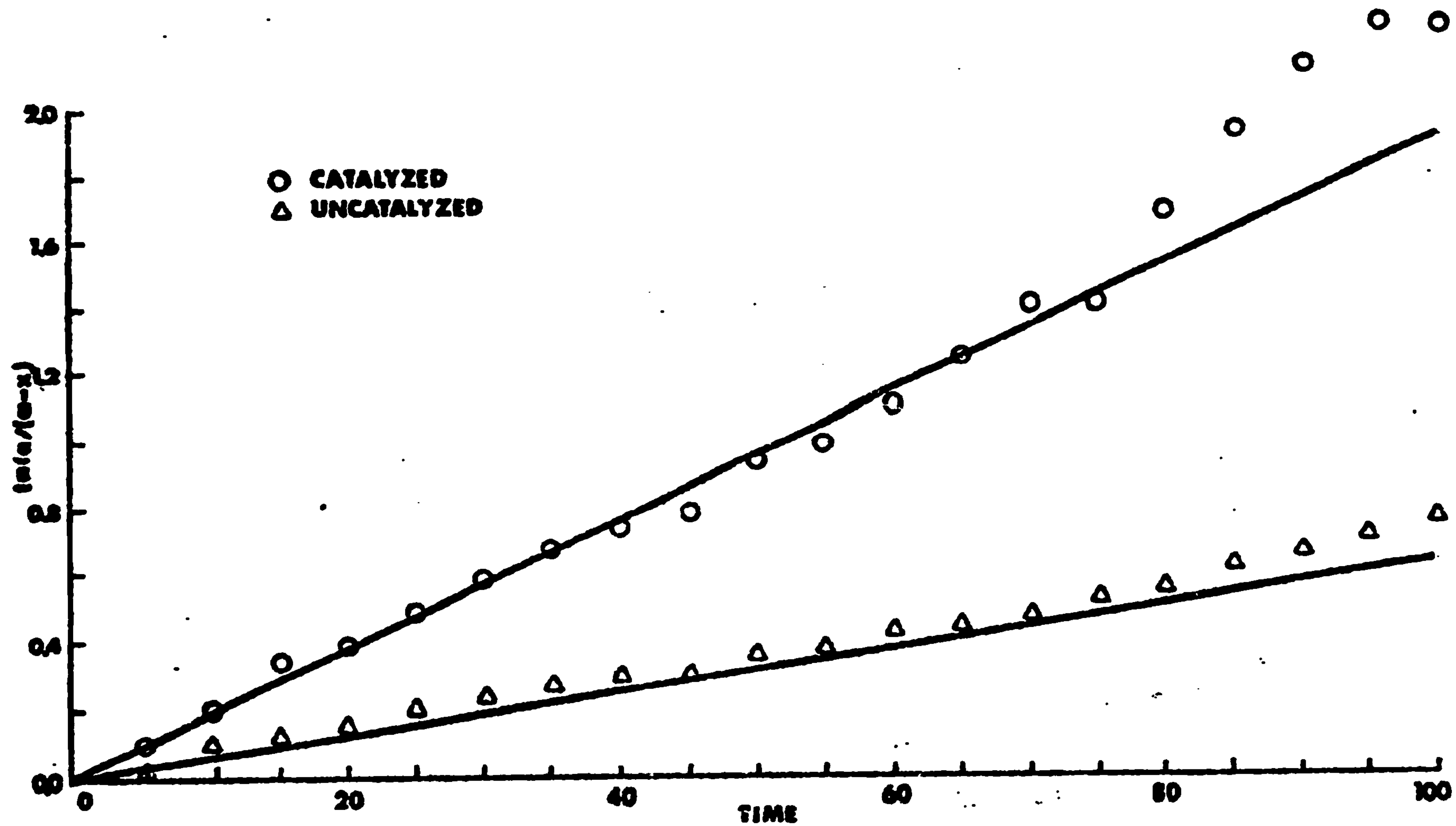


FIGURE 5
DEPENDENCE OF ln(a/(a-x)) UPON TIME FOR CHEMICAL
AND MCIC SIMULATED FIRST-ORDER CATALYZED
AND UNCATALYZED PROCESSES

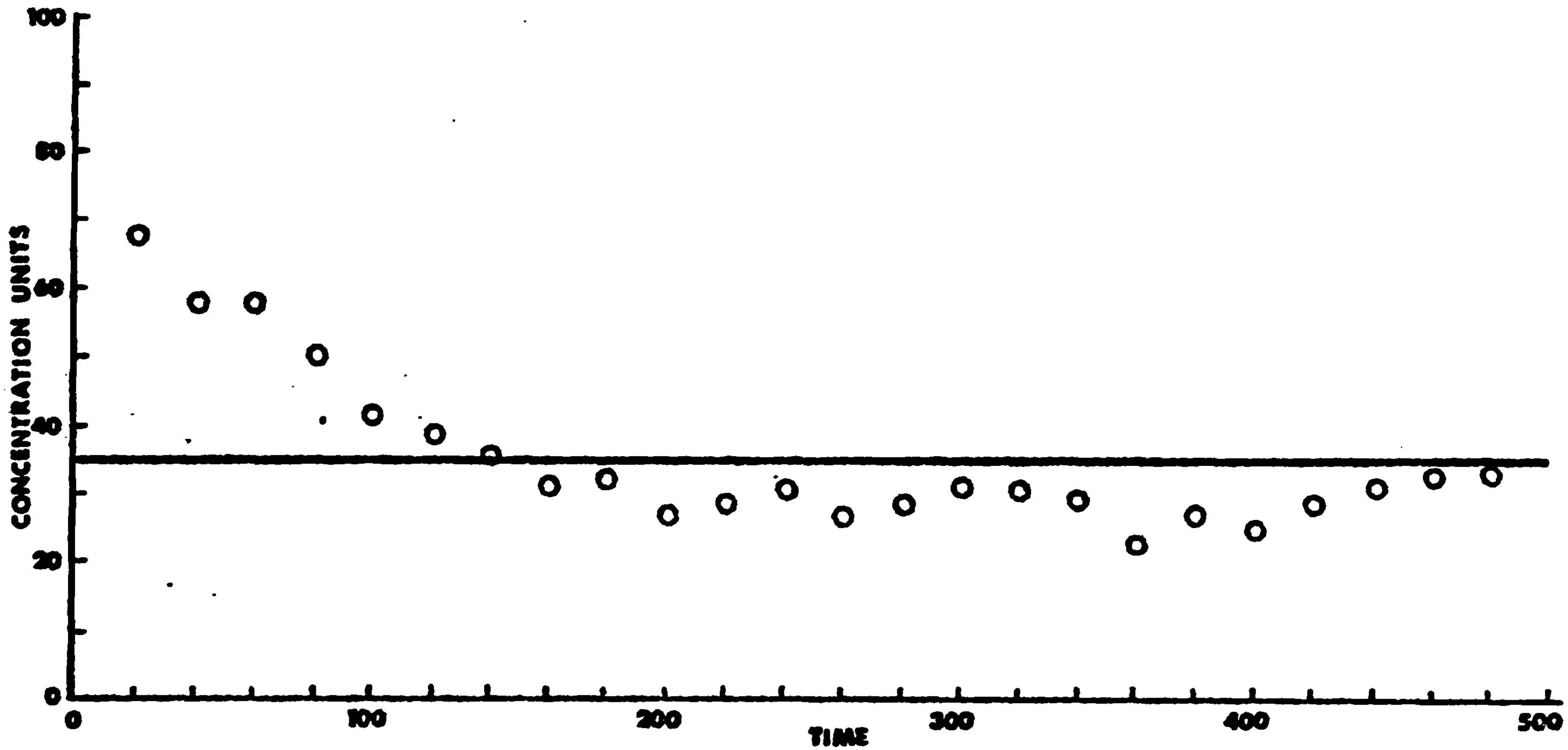


FIGURE 6
DEPENDENCE OF REACTANT CONCENTRATIONS UPON TIME FOR CHEMICAL AND MCIC SIMULATED EQUILIBRIUM PROCESSES OF THE FORM A+B⇌C

EVALUATION

Determination of Appropriate Evaluative Design

An aspect of this study that may be of particular interest to the NARST membership is the procedure used for evaluating the MCIC as an instructional aid. Summative educational research procedures were initially contemplated. However, such procedures appear to have been of limited usefulness in the past for evaluating instructional aids. Lumsdaine made the following comments:

> Experimental measurement of the effects of a single instrument apply only to that particular instrument, and generalizations of the results of such an evaluative experiment to other instruments of the media it represents have, at most, the status of untested hypotheses. Similar limitations apply when a comparison is made between the attainments affected by a particular instrument and those obtained by some alternative form of instruction often characterized as "conventional" or "currently used" instruction. The restrictions on interpretation of such a comparison arise from the lack of specificity of the instruction with which the instrument in question is compared. Similar restrictions apply in general to the overall comparison of alternative "media." (Glaser, R., Training Research in Education. New York: Science Editions, John Wiley and Sons, Inc. page 251, 1965)

In addition, Jacobson stated:

> Teachers and instructional leaders have to make decisions as to the choice of materials and procedures, and it would be desirable to have these decisions based upon research. It is difficult, and usually suspect, for the developers to undertake this kind of evaluation research .... In many cases, it may be more desirable to have school systems and other consumers evaluate innovations by undertaking systematic pilot tests of innovations under local conditions. (Jacobson, W. J., Approaches to Science Education Research: Analysis and Criticism. Paper presented at the Annual Luncheon Meeting of the National Association for Research in Science Teaching, Leamington Hotel, Minneapolis, Minnesota, March 7, 1970.)

Absolute or comparative summative research procedures were therefore considered by this researcher to be of minimal usefulness for both the evaluation of the MCIC and as a source of knowledge related to instructional aids in general. Therefore, these avenues for evaluating the MCIC were not further pursued.

Lumsdaine, Flanagan and others have suggested alternative "formative" procedures that appear to have much merit for evaluating the MCIC and other instructional aids. Lumsdaine states:

> An important class of evaluative experiments includes those which are conducted for what may be called "diagnostic" purposes, in which specific effects of the instrument of a <u>number of specific points</u> relating to its objectives are separately measured . . . . The results can then be used in modifying or redesigning the instrument so as to correct or strengthen its weak points. (Glaser, Ibid)

<u>Diagnostic Evaluation of the MCIC</u>

Lumsdaine's suggested procedure was implemented through the development of a diagnostic or formative evaluation of the MCIC. Diagnostic questions, diagnoses, and remedial procedures were linked in a manner to provide on-going evaluation and feedback. The evaluation occurred over three lecture-demonstration presentations of the MCIC to Philadelphia area high school chemistry students. The diagnostic model for evaluating the MCIC is shown in Figure 7. Diagnostic questions, diagnoses and remedial procedures used within a given problem

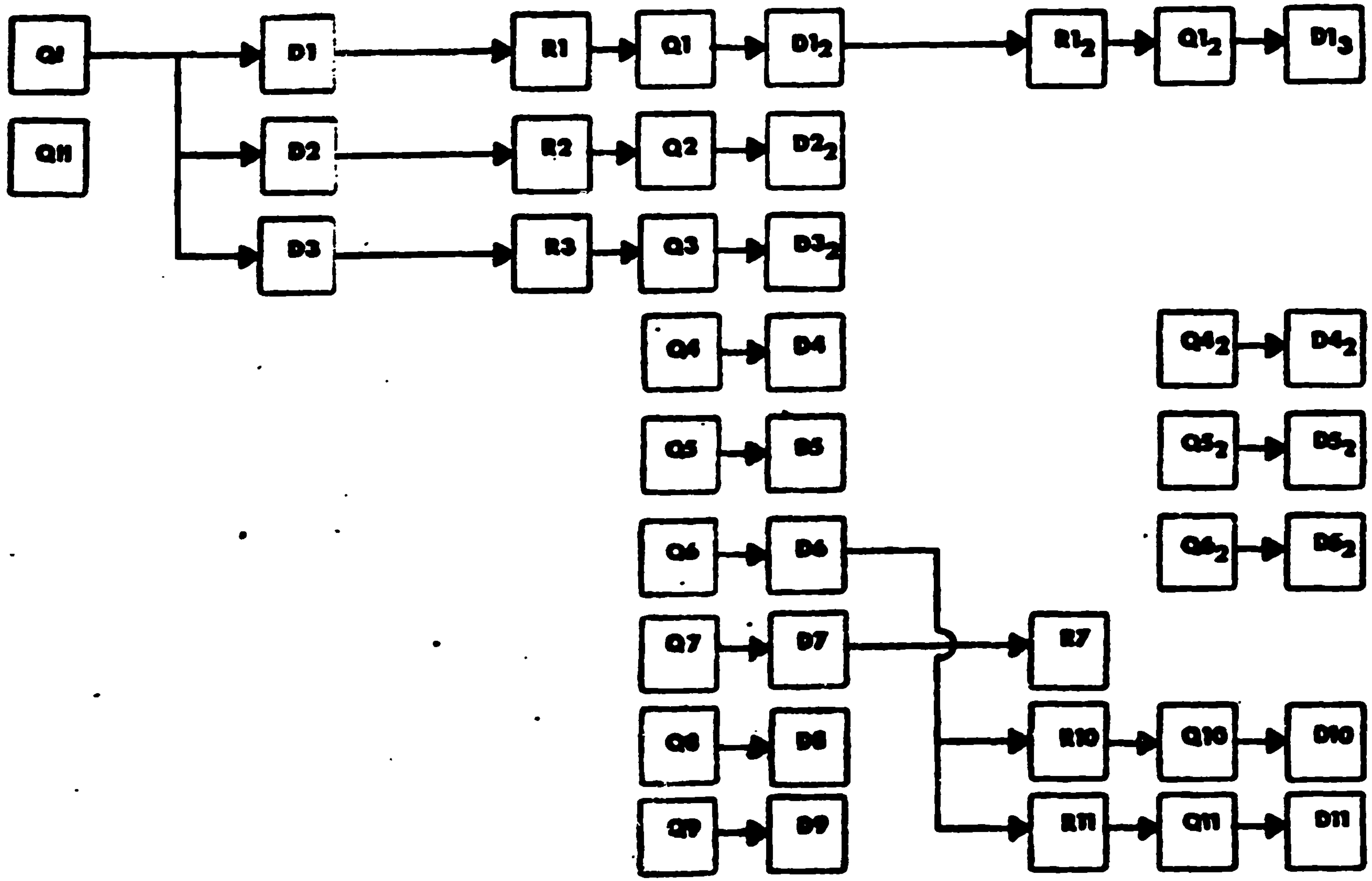


FIGURE 7

DIAGNOSTIC MODEL FOR EVALUATING THE MCIC area are depicted by horizontally aligned rectangles. Within this figure the symbol "Q" represents a diagnostic question, "D" represents a diagnosis, and "R" represents a remedial procedure. The numeral subscripts indicate the number of times that a question, diagnosis or remedial procedure had been utilized within a given problem area.

The purpose of this portion of the report is not to elucidate specific findings related to the MCIC but rather to communicate the potential usefulness of this particular evaluation model. Thus, findings obtained from only one problem area will be reported to provide an example of the characteristics of the evaluation model.

During the initial pilot presentation of the MCIC, a question (QI) was used to probe possible pedagogical difficulties related to the MCIC and its presentation. This question asked: "In what ways was the lecture-demonstration of the MCIC confusing or hard to understand?" From eleven student responses the following diagnosis and two others were obtained.

> Diagnosis D1: Some students expressed difficulty in relating simulated first-order processes to chemical reactions that involve single species. The difficulty appeared to stem from much emphasis that had been placed upon bimolecular reaction mechanisms within the classes.

In preparation for the second presentation of the MCIC to a different group of high school chemistry students, the following remedial procedure was implemented.

Remedial Procedure R1: Demonstration Experiment materials were carefully constructed to provide adequate explanation and illustration of first-order reaction processes. A more direct remedial procedure involving the replacement of MCIC simulated single-species processes with two-species processes was not undertaken dur to the increased complexity of the second-order rate law to high school students.

A diagnostic questionnaire was presented to this second group of students after their participation in the lecture-demonstration of the MCIC. The following diagnostic question was presented to determine the effectiveness of remedial procedure R1.

Diagnostic Question Q1: Would you have understood the demonstration better if "A" had reacted with "B" to produce "C" rather than to have had "A" react with itself?

This question is related, of course, to the process whereby a given species is the sole reactant, as for example with radioactive decay. Evaluation of forty-five responses to the questionnaire led to the following diagnosis:

Diagnosis $D1_2$: Forty-seven percent of the students responding to question Q1 indicated no preference for simulated two-species reactions over one-species reactions. However, forty-two percent of the students did indicate a preference for the simulation of a two-species reaction. Remedial procedure R1 appears to be indecisive.

The third presentation of the MCIC to high school chemistry students incorporated the remedial procedure $R1_2$ listed below.

Remedial Procedure $R1_2$: Demonstration Experiment III was constructed to include the MCIC simulation of two-species processes. An effort was made to minimize the mathematical aspects of the presentation.

A diagnostic questionnaire was presented to the third group of students after having participated in the lecture-demonstration of the MCIC. The following diagnostic question was included to determine the effectiveness of remedial procedure Rl_2:

> Diagnostic Question Ql_2: Would you have understood the demonstration better if "A" had reacted with itself to produce "C" rather than having "A" react with "B" to produce "C"?

Evaluation of one hundred forty-seven responses to the diagnostic questionnaire led to the following diagnosis.

> Diagnosis Dl_3: Five, eight, and eighty-seven percent of the students responded in a positive, neutral and negative manner respectively to question Ql_2. Mixed student responses were obtained from previous demonstration experiments that utilize the MCIC simulation of first-order processes. A clear preference was obtained, however, for the third demonstration experiment that utilized the simulation of two-species reaction processes. The simulation of two-species processes is therefore considered to be preferable over one-species processes for demonstration to contemporary high school students.

Conclusion:

In light of the utility of findings obtained within this study as is indicated in the above example, and also of the questionable usefulness of data obtained through summative evaluation of instructional aids, this reporter is suggesting that evaluators of instructional aids and materials seriously consider formative evaluation as a fruitful alternative to the "good-better-best" research of the past.